Xiaoyu Wang

Postdoctoral Appointee
Chemistry Sciences and Engineering Division
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EDUCATION

Bachelor of Science: Applied Chemistry 2008—2012

Sichuan University, Chengdu, Sichuan Province, China

Master of Engineering: Chemical Engineering 2013—2015

Illinois Institute of Technology, Chicago, IL, U.S.

Doctor of Philosophy: Chemical Engineering 2015—2020

Illinois Institute of Technology, Chicago, IL, U.S.

PhD Dissertation Title: "Using Computational Molecular Modeling to Study Transport Processes of Interest in Separations"

Dissertation Advisor: Dr. Sohail Murad; Dr. Cynthia J. Jameson

RESEARCH EXPERIENCE

Postdoctoral Research Associate 05/2020 - Present

University of Notre Dame, Notre Dame, IN, U.S.

Role: To develop and utilize molecular dynamics simulations to understand how additives affect the thermophysical properties of deep eutectic solvents and to use simulations to understand how templating agents affect the performance of zeolite catalysts.

Graduate Research Assistant 05/2015 - 05/2020

Illinois Institute of Technology, Chicago, IL, U.S.

Role: To investigate chiral drug separation processes on polysaccharide-based polymer surfaces; to study fluid separations through zeolite membranes and provide insights when separations fail; to use molecular dynamics simulations to characterize the anisotropy of thermal conductivity at interfaces.

NSF Funded Industrial Internship 09/2017—03/2018

Orochem Technologies, Inc, Naperville, IL, U.S.

Role: To use molecular simulations to increase the efficiency of industrial separations; to work with employees to help to facilitate SBIR project between IIT and Orochem Tech; to develop a software prototype for enantio-separation of chiral drugs.

Undergraduate Research Assistant 09/2011 - 05/2012

Sichuan University, Chengdu, Sichuan Province, China

Role: To synthesis and characterize organic fluorescent materials.

TEACHING EXPERIENCE

Teaching Assistant 06/2015—08/2015

Illinois Institute of Technology, Chicago, IL, U.S.

Role: Supervised and guided laboratory work in fluid flow, heat transfer, distillation, humidification, drying, gas absorption, filtration, etc. in an undergraduate Unit Operations course in Chemical Engineering.

Undergraduate Research Mentor Summer, 2021

University of Notre Dame, Notre Dame, IN, U.S.

Role: Trained summer graduate student on how to use molecular dynamics simulations to model ionic liquids and other systems of interest.

SCIENTIFIC COMMUNITY AND OUTREACH ACTIVITIES

Proposal Preparations

- The Icelandic Research Fund (2022): Biochirality of usnic acid enantiomers in lichens (ChiralLichen).
- Air Liquid Project: Conversion of Ortho to Para Hydrogen.
- NSF: Using Machine Learning Technology to Extract and Study Phenomena That Are Not Well Understood in Molecular Modeling Simulations.
- GOALI: Molecular Dynamics Simulations for Prediction of Separation Factors for a Polysaccharide Chiral Stationary Phase in Enantiomeric Chromatographic Separations

Manuscript Reviews

- Adsorption.
- The Journal of Physical Chemistry
- Molecular Simulation
- Fluid Phase Equilibria
- Separation and Purification Technology
- Computational Materials Science
- Australian Journal of Chemistry
- Colloids and Surfaces A: Physicochemical and Engineering Aspects
- Results in Chemistry

AWARDS & HONORS

5. NSF Graduate Research Fellowship, Illinois Institute of Technology, 2015
4. Gamson Fellowship, Illinois Institute of Technology, 2014
3. Energy Technology Fellowship, Illinois Institute of Technology, 2013
2. Excellent Undergraduate Award, Sichuan University, 2010
1. Excellent Undergraduate Award, Sichuan University, 2009

PUBLICATIONS

17. Maonian Xu, Ernest Oppong-Danquah, **Xiaoyu Wang**, Sebastian Oddsson, Asmaa Abdelrahman, Simon Vilms Pedersen, Maria Szomek, Aron Elvar Gylfason, Bergthora Sigridur Snorradottir, Eva Arnspang Christensen, Deniz Tasdemir, Cynthia J Jameson, Sohail Murad, Olafur Sigmar Andresson, Kristinn Petur Magnusson, Hugo J de Boer, Margret Thorsteinsdottir, Sesselja Omarsdottir, Starri Heidmarsson, Elin Soffia Olafsdottir "Novel methods to characterise spatial distribution and enantiomeric composition of usnic acids in four Icelandic lichens" Phytochemistry 2022, Vol. 200, 113210

16 Bandar J. Bashmmakh, **Xiaoyu Wang**, Cynthia J. Jameson and Sohail Murad "Understanding Separation Mechanisms of Monoatomic Gases, Such as Kr and Xe, via DD3R Zeolite Membrane Using Molecular Dynamics" Thermo 2 (1), 56-73

15. **Xiaoyu Wang**, Yujia Wang, Edward Maginn, William Schneider "Using Molecular Modeling Methods to Predict the Aluminum Distribution in the Chabazite Zeolite with the Presence of Organic Structure Directing Agents" arXiv:2110.12523

14. Derrick Poe, **Xiaoyu Wang**, Yong Zhang, Jeffery Klein, William Dean, Burcu Gurkan, and Edward J. Maginn, "A Systematic Study of Deep Eutectic Solvents Composed of Choline Chloride and Phenol Derivatives: A Combined Study of Experimental and Molecular Dynamics Simulation Methods" (in preparation)

13. Mufarreh Asmari, **Xiaoyu Wang**, Natalia Casado, Marjan Piponski, Sergiy Kovalenko, Liliya Logoyda, Rasha Sayed Hanafi, and Sami El Deeb. "Chiral Monolithic Silica-Based HPLC Columns for Enantiomeric Separation and Determination: Functionalization of Chiral Selector and Recognition of Selector-Selectand Interaction." Molecules 2021, 26, 5241

12. **Xiaoyu Wang**, Cynthia J Jameson, Sohail Murad, "Molecular dynamics simulations of chiral recognition of drugs by amylose polymers coated on amorphous silica" Molecular Physics 2021, Vol. 119, e1922772

11. Cynthia J Jameson, **Xiaoyu Wang**, Sohail Murad, "Molecular Dynamics Simulations of Enantiomeric Separations as an Interfacial Process in HPLC" AIChE Journal 2021, 67, e17143

10. **Xiaoyu Wang**, Cynthia Jameson, Sohail Murad, "Modeling enantiomeric separations as an interfacial process using amylose tris(3,5-dimethylphenyl carbamate) (ADMPC) polymers coated on amorphous silica" Langmuir 2020, 36, 1113-1124

9. **Xiaoyu Wang**, Cynthia Jameson, Sohail Murad, "Interfacial Thermal Conductivity and its Anisotropy" Processes 2020, 8, 27

8. **Xiaoyu Wang**, David Venerus, Ishwar Puri, Sohail Murad, "On Using the Anisotropy in the Thermal Resistance of Solid-Fluid Interfaces to More Effectively Cool Nano-electronics" Molecular Simulation 2020, 46, 162-167

7. Xuerui Wang, Yuting Zhang, **Xiaoyu Wang,** Eduardo Andres-Garcia, Peng Du, Lorena Giordano, Lin Wang, Zhou Hong, Xuehong Gu, Sohail Murad, Freek Kapteijn, "Xe Recovery by DD3R Zeolite Membranes - Application in Anaesthetics" Angewandte Chemie International Edition 2019, 58, 15518-15525

6. **Xiaoyu Wang**, David House, Priyanka Oroskar, Anil Oroskar, Asha Oroskar, Cynthia Jameson, Sohail Murad, "Molecular Dynamics Simulations of the Chiral Recognition Mechanism for a Polysaccharide Chiral Stationary Phase in Enantiomeric Chromatographic Separations" Molecular Physics 2019, 117, 3569-3588

5. Kevin Hinkle, **Xiaoyu Wang**, Xuehong Gu, Cynthia Jameson, Sohail Murad, "Computational Molecular Modeling of Transport Processes in Nanoporous Membranes" Processes 2018, 6, 124

4. Chuan Chen, Yuli Cheng, Li Peng, Chun Zhang, Zhengqi Wu, Xuehong Gu, **Xiaoyu Wang**, Sohail Murad "Fabrication and stability exploration of hollow fiber mordenite zeolite membranes for isopropanol/water mixture separation" Microporous and Mesoporous Materials 2019, 274, 347-355

3. **Xiaoyu Wang**, Sohail Murad, "Molecular dynamics simulations of liquid-liquid phase equilibrium of ternary methanol/water/hydrocarbon mixtures" Fluid Phase Equilibria 2018, 470, 109-119

2. Binwu Zhao, Priyanka Sharma, **Xiaoyu Wang**, David House, Anil Oroskar, Asha Oroskar, Cynthia Jameson, Sohail Murad, "Computational study on chiral recognition of drug molecules" Langmuir 2017, 33, 11246-11256

1. Fanyu Qu, Rui Shi, Li Peng, Yuting Zhang, Xuehong Gu, **Xiaoyu Wang**, Sohail Murad, "Understanding the Effect of Zeolite Crystal Expansion/Contraction on Separation Performance of NaA Zeolite Membrane: A Combined Experimental and Molecular Simulation Study" Journal of Membrane Science 2017, 539, 14-23

CONFERENCES

12. "583b Combining Ab Initio and Classical Molecular Dynamics Simulations to Predict the Implication of Charged OSDAs on of Al Siting Preferences in CHA." Catalysis and Reaction Engineering Division, Nov. 11, 2021, AIChE 2021 Annual Meeting, Boston, MA.
11. "451c Tuning Deep Eutectic Solvent Properties with Phenolic-Derivative Hydrogen Bond Donors." Thermodynamics and Transport Properties, Nov. 10, 2021, AIChE 2021 Annual Meeting, Boston, MA.
10. "383c Interfacial Thermal Conductivity and Its Anisotropy." Transport Processes, Nov. 9, 2021, AIChE 2021 Annual Meeting, Boston, MA.
9. "412g Molecular Dynamics Simulations of Enantiomeric Separations As an Interfacial Process in HPLC." Adsorption and Ion Exchange, Nov. 8, 2021, AIChE 2021 Annual Meeting, Boston, MA
8. "4ez Using Atomistic Simulations and Machine Learning Technology to Discover New Porous Materials for Sustainable Energy Applications." Nov. 7, 2021, AIChE 2021 Annual Meeting, Boston, MA.
7. "Using Molecular Simulations to Understand the Structure and Properties of Deep Eutectic Solvents, With Application to Flow Batteries." V CINE-CMSC Workshop, Sao Carlos Institute of Chemistry, University of Sao Paulo, Sao Carlos, Brazil (Derrick Poe, Yong Zhang, **Andy Wang**, and Edward Maginn)
6. "On Using the Anisotropy in the Thermal Resistance of Solid-Fluid Interfaces to More Effectively Cool Nano-electronics." Fundamental Research in Transport Processes, November 12, 2019, AIChE Annual Meeting, Orlando, FL. (co-authors: David Venerus, Ishwar Puri, Sohail Murad)
5. "Molecular simulations of separations of enantiomer using chiral stationary phases." Division of Colloid and Surface Chemistry, March 31st, 2019, ACS Spring 2019 National Meeting, Orlando, FL. (co-authors: Priyanka Sharma, Cynthia Jameson, Sohail Murad)
4. "Molecular dynamics simulations of liquid-liquid phase equilibrium of ternary methanol/water/hydrocarbon mixtures" March 14th, 2018, AIChE Midwest Regional Conference, Chicago. (co-author: Sohail Murad)
3. "Molecular Modeling as a Screening Tool to Separate Enantiomers of Chiral Compounds Using Polysaccharide-based Chiral Stationary Phases for Orphan Drugs" Feb 28th, 2017, AIChE Midwest Regional Conference, Chicago. (co-authors: Binwu Zhao, Priyanka Sharma, Cynthia Jameson, Sohail Murad)
2. "Molecular Modeling of Liquid-Liquid Phase Equilibria in Ternary Systems" March 1st, 2017, AIChE Midwest Regional Conference, Chicago. (co-author: Sohail Muard)
1. "Effect of Linear Hexane on Dehydration of Isopropanol-Water mixture through NaA Zeolite Membranes" March 3rd, 2016, AIChE Midwest Regional Conference, Chicago. (co-author: Sohail Murad)